An analysis of the $t_2 - V$ (or extremely anisotropic next-nearest-neighbor Heisenberg) model

A. Ghosh[1] and S. Yarlagadda[1,2]
[1] *TCMP Div., Saha Institute of Nuclear Physics, Kolkata, India and*
[2] *Cavendish Lab, Univ. of Cambridge, Cambridge, UK*

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The $t_2 - V$ model (involving next-nearest-neighbor hopping and nearest-neighbor repulsion) has been shown to depict the limiting case of strong electron-phonon coupling in a molecular chain with cooperative breathing mode [R. Pankaj and S. Yarlagadda, Phys. Rev. B **86**, 035453 (2012)]. Our $t_2 - V$ model can be mapped onto an extremely anisotropic Heisenberg model (with next-nearest-neighbor XY interaction and nearest-neighbor ising interaction) and is of the form $J_\perp \sum_i (S^+_{i-1} S^-_{i+1} + \text{H.c.}) + J_\parallel \sum_i S^z_i S^z_{i+1}$. Using finite size scaling, at non-half-fillings of the $t_2 - V$ model (or non-zero magnetizations of the spin model), we numerically obtain the critical repulsion for a quantum phase transition by using modified Lanczos method. During the transition, away from half-filling (zero magnetization), the system undergoes a striking discontinuous transition from a superfluid to a supersolid [i.e., a superfluid homogeneously coexisting with a period-doubling charge-density-wave (antiferromagnetic) state]. At half-filling, the charge-density-wave (Néel) state and the superfluid state are mutually exclusive. We also derive microscopically, using Green's functions, the exact instability conditions in the two limiting cases of the $t_2 - V$ model for hard-core-bosons: the two-particle system and the half-filled system. We show explicitly that the critical repulsion V_c for the two-particle case is $V_c/t_2 = 4$ for a ring of any size while for the half-filled case the $V_c/t_2 = 2\sqrt{2}$ in the thermodynamic limit. Our spin model correspondingly lends itself to exact instability solutions (by the Green's function method) in the two limiting cases of two-magnons (the non-trivial highest excited state) and Néel antiferromagnet ground state.

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I. INTRODUCTION

The cooperation or competition between diagonal charge/spin long range orders and superfluid/superconductor off-diagonal long range orders in electronic phases leading to coexistence or mutual exclusivity of these orders is a subject of active current interest. Coexistence of charge-density-wave (CDW) and superconductivity/superfluidity is manifested in various systems with differing dimensions: helium-4[2], bismuthates (e.g., $BaBiO_3$ doped with K or P)[3], non-iron based pnictides (e.g., $SrPt_2As_2$)[4], layered dichalogenides (e.g., 2H-$TaSe_2$, 2H-TaS_2, and $NbSe_2$)[5], quasi-one-dimensional trichalcogenide $NbSe_3$[6] and doped spin ladder cuprate $Sr_{14}Cu_{24}O_{41}$[7], etc.

A number of materials indicate strong electron-phonon (e-ph) interactions along with the larger energy scale electron-electron (e-e) interactions. For instance, oxides such as cuprates[8–10], manganites[11–13], and bismuthates[14] indicate strong e-ph coupling. The coaction of e-e and e-ph interactions in these correlated systems leads to coexistence of or incompatibility between various phases such as superconductivity, CDW, etc.

Many oxides have a perovskite structure with the formula ABO_3; they have two adjacent BO_6 octahedra sharing an oxygen which leads to cooperative octahedral distortions. Examples of simple three-dimensional systems exhibiting cooperative breathing-mode (CBM) phenomena are the barium bismuthates ($BaBiO_3$) where $Bi - O$ bonds of adjacent octahedra differ by about 10%[14]. Next, copper oxides[15,16] can be modeled as a one-band two-dimensional CBM system with the copper onsite energy being modulated by the movement of adjacent oxygen closer to or further from it[15,16]. Lastly, in manganite systems when C-type antiferromagnetism manifests [as in $La_{1-x}Sr_xMnO_3$ for $0.65 \leq x \leq 0.9$[17]], the d_{z^2} orbitals participate in the C-chain ordering; the ferromagnetic C-chain is a one-band (involving d_{z^2} orbitals) one-dimensional CBM system.

Earlier, we showed that cooperative effects in a one-dimensional CBM system change its dominant transport from a nearest-neighbor (NN) hopping mechanism to that of a next-nearest-neighbor (NNN) hopping[1]. Additional NN particle repulsion (due to incompatibility of NN breathing-mode distortions) leads to the $t_2 - V$ model as the effective model for the 1D CBM model.

In this paper, upon tuning repulsion, we show that the $t_2 - V$ model undergoes a dramatic discontinuous transition from a superfluid state to a supersolid state (involving superfluidity in one sub-lattice only). We find that (instead of competing for the Fermi surface), the superfluid and the CDW coexist. Using Green's functions, we derive the exact critical repulsion V_c in two limiting cases; we find $V_c = 4t_2$ for the two-particle system and $V_c = 2\sqrt{2}t_2$ for the half-filled system. Using finite size scaling analysis [with $V_c(N) - V_c(\infty) \propto 1/N^2$ for system size N], we also obtain the critical repulsion at other fillings numerically by using modified Lanczos algorithm[18].

Our $t_2 - V$ model can be mapped onto an extremely anisotropic Heisenberg model (with next-nearest-neighbor XY interaction and nearest-

neighbor ising interaction) and is of the form $J_\perp \sum_i (S_i^+ S_{i+2}^- + H.c.) + J_\parallel \sum_i S_i^z S_{i+1}^z$. While Heisenberg model was amenable to solution through the Bethe ansatz, the addition of next-nearest-neighbor interaction requires an alternate route for its solution. Thus, the Majumdar-Ghosh model[19] $(J\sum_i[\vec{S}_i\cdot\vec{S}_{i+1} + \frac{1}{2}\vec{S}_i\cdot\vec{S}_{i+2}])$, which is a special case of the isotropic Heisenberg model with nearest- and next-nearest-neighbor coupling, can be solved by an alternate elegant approach yielding an exact ground state cast in a simple valence-bond form. Our spin model too lends itself to exact instability solutions (by the Green's function method) in the two limiting cases of two-magnons and antiferromagnetic ground state.

II. NUMERICAL STUDY OF THE $t_2 - V$ MODEL

We begin by identifying the Hamiltonian of the $t_2 - V$ model for hard-core-bosons (HCB).

$$H_{t_2V} \equiv -t_2 \sum_{j=1}^{N} (b_{j-1}^\dagger b_{j+1} + \text{H.c.}) + V \sum_{j=1}^{N} n_j n_{j+1}, \quad (1)$$

where b_j is destruction operator for a HCB, $V \geq 0$, $n_j = b_j^\dagger b_j$, and N (which is even) is the total number of sites. We will study numerically the quantum phase transition (QPT) in the $t_2 - V$ model by assuming periodic boundary conditions. We will characterize the transition through the structure factor and the superfluid density. The structure factor is given by

$$S(k) = \sum_{l=1}^{N} e^{ikl} W(l), \quad (2)$$

where $W(l)$ is the two-point correlation function for density fluctuations of HCBs at a distance l apart (when lattice constant is set to unity),

$$W(l) = \frac{4}{N} \sum_{j=1}^{N} \left[\langle n_j n_{j+l}\rangle - \langle n_j\rangle\langle n_{j+l}\rangle\right], \quad (3)$$

wavevector $k = \frac{2n\pi}{N}$ with n=1,2,.....,N; filling-fraction $f \equiv \langle n_j\rangle = \frac{N_p}{N}$ with N_p being the total number of HCBs in the system. Now, we observe that $\hat{N}_e = \sum_{j_{\text{even}}} n_j$ ($\hat{N}_o = \sum_{j_{\text{odd}}} n_j$) the number operator which gives the total number of electrons at even (odd) sites commutes with the Hamiltonian; hence the following simple expression results[1]

$$S(\pi) = \frac{4\langle(\hat{N}_e - \hat{N}_o)^2\rangle}{N} = \frac{4(N_e - N_o)^2}{N}, \quad (4)$$

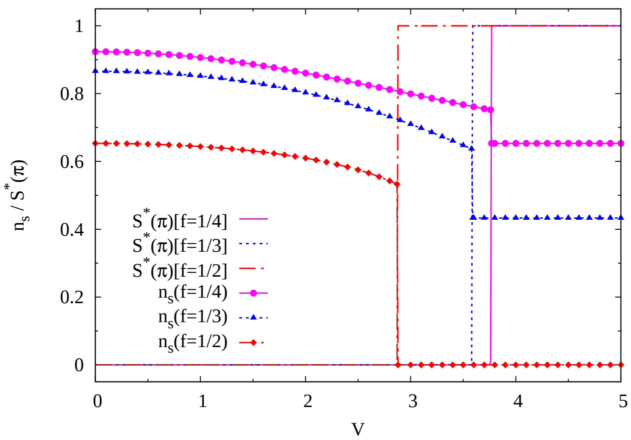

FIG. 1. (Color online) Plots of rescaled structure factor $S^*(\pi)$ and superfluid fraction n_s at various filling factors f obtained using modified Lanczos technique. The calculations were performed at fillings f $= 1/2, 1/4$ with system size $N = 16$ while at f $= 1/3$ size $N = 12$ was used. At a critical repulsion there is a striking discontinuous transition in both $S^*(\pi)$ and n_s; while $S^*(\pi)$ jumps from its minimum to maximum, there is a significant drop in n_s.

where N_e (N_o) are the number of HCBs in even (odd) sites. Thus the minimum value of $S(\pi) = 0$ corresponds to equal number of particles in both the sub-lattices whereas the maximum is given by

$$[S(\pi)]_{\max} = \frac{4N_p^2}{N}, \quad (5)$$

indicating a single sublattice occupancy. To study the QPT, we rescale the value of $S(\pi)$ as follows:

$$S^*(\pi) = \frac{S(\pi)}{[S(\pi)]_{\max}}, \quad (6)$$

with $S^*(\pi)$ representing the order parameter that varies from 0 to 1 during the phase transition.

Next, we will outline our procedure for calculating the superfluid density by threading the chain with an infinitesimal magnetic flux θ. The superfluid fraction is given by[20,21]

$$n_s = \frac{N^2}{N_p t_{eff}} \left[\frac{1}{2}\frac{\partial^2 E(\theta)}{\partial\theta^2}\right]_{\theta=0}, \quad (7)$$

where $E(\theta)$ is the total energy when threaded by flux θ and $t_{\text{eff}} = \hbar^2/2m$ is the effective hopping term which for our $t_2 - V$ model is given by $t_{\text{eff}} = 4t_2$. The total energy for the case $V = 0$ when threaded by a flux θ, is expressed as

$$E(\theta) = -2t_2 \sum_k \cos[2(k + \theta/N)]. \quad (8)$$

When, both sub-lattices are occupied, the superfluid fraction is given by[22]

$$n_s = \frac{2}{N_p} \frac{\sin\left(\frac{\pi N_p}{N}\right)}{\sin\left(\frac{2\pi}{N}\right)}, \quad (9)$$

whereas when only one sub-lattice is occupied it is expressed as

$$n_s = \frac{1}{N_p} \frac{\sin\left(\frac{2\pi N_p}{N}\right)}{\sin\left(\frac{2\pi}{N}\right)}, \tag{10}$$

where periodic boundary conditions have been taken.

Here, we do not calculate the Bose-Einstein condensate (BEC) occupation number n_0 because, for a system of HCB in a one-dimensional tight-binding lattice, it varies as $C(\mathrm{f})\sqrt{N}$ in the thermodynamic limit with the coefficient $C(\mathrm{f})$ depending on filling fraction f[23,24]; consequently, the condensate fraction $n_0/N_p \propto 1/\sqrt{N} \to 0$. Next, in the presence of repulsion (as argued in Ref. 22), we expect the BEC occupation number n_0 to again scale as $\sqrt{N}$; however, the coefficient of $\sqrt{N}$ will be smaller due to the restriction on hopping imposed by repulsion.

When rings with even number of sites were used, at all fillings f, we found that the order parameter $S^*(\pi)$ jumps from 0 to 1 at a critical value of repulsion V_c indicating that the system transits from equally populated sub-lattices (i.e., ising symmetry) case to a single sub-lattice occupancy, i.e., a period-doubling CDW state [see Fig. (1)]. Concomitantly, as can be seen from Fig. (1), there is a sudden drop in the superfluid fraction n_s at the same critical repulsion. At half-filling, where the superfluid fraction vanishes above a critical repulsion because a single sub-lattice is completely filled, the transition shows that superfluidity and CDW state are mutually exclusive. On the other hand, at all non-half-fillings, we see that the system undergoes a QPT from a superfluid to a supersolid (i.e., a homogeneously coexisting superfluid and CDW) state. In Fig. (1), it is of interest to note that the values of n_s at $V = 0$ and $V > V_c$ are exactly those predicted by Eq. (9) and Eq. (10) respectively.

Next, using the finite size scaling expression (as derived in Appendix A) relating $V_c(N)$ (critical repulsion at a finite N) to $V_c(\infty)$ (critical repulsion of an infinite system)

$$V_c(N) - V_c(\infty) = \frac{A}{N^2} + \frac{B}{N^4} + ..., \tag{11}$$

we obtain the critical $V_c(\infty)$ depicted in Fig. (2) (from finite size systems calculations) at various fillings. At half-filling, from finite size scaling analysis we obtain that $V_c(\infty) \approx 2.83$; in the next section, we show (using Green's function analysis) the exact result $V_c(\infty) = 2\sqrt{2}$. For systems with 2 HCB and $N = 4, 6, 8, 10, 12, 14, 16, 18,$ and 20, we find numerically that $V_c \approx 4.00$; in the next section, we obtain the exact result (using Green's functions) that $V_c(N) = 4$ for any system size $N \geq 4$. We will now cast the $t_2 - V$ model (for HCBs) as an extremely anisotropic Heisenberg spin model by identifying $S^+ = b^\dagger$, $S^- = b$, and $S^z = n - \frac{1}{2}$. The resulting spin Hamiltonian is of the form

$$-t_2 \sum_{i=1}^{N} (S^+_{i-1} S^-_{i+1} + \text{H.c.}) + V \sum_{i=1}^{N} S^z_i S^z_{i+1}. \tag{12}$$

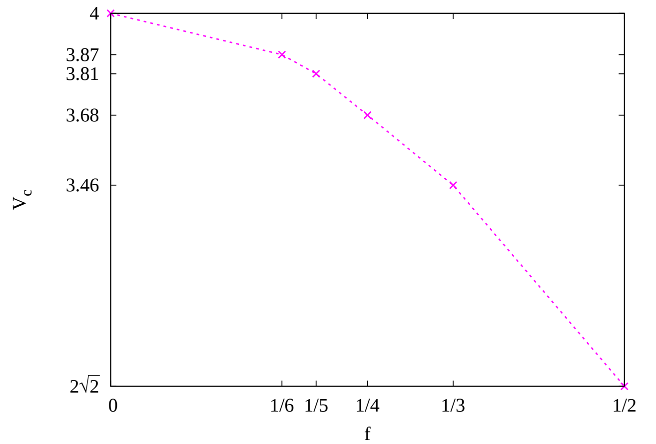

FIG. 2. (Color online) Plot of $V_c(\infty)$ (critical repulsion for an infinite system) obtained from Green's function analysis for half-filled (f = 1/2) and two HCB systems (f → 0) and using finite size scaling at various other fillings f.

We see that the above spin model has NNN interaction in the transverse (XY) channel while it has NN interaction in the longitudinal (Z) channel. The energies at various fillings N_p/N for the $t_2 - V$ model correspond to various magnetizations $(N - 2N_p)/N$ for the spin model. From a plot of the energies at various magnetizations of the spin model, as depicted in Fig. (3), we see that the energy increases with magnetization with the ground state corresponding to zero magnetization. From the fact that always the critical repulsion $V_c \leq 4$, it should be clear that the energy at all fillings and system sizes for $V_c > 4$ is obtained from a tight-binding model with N_p particles in one sub-lattice only. Thus at $V_c > 4$, the energy will certainly increase with magnetization.

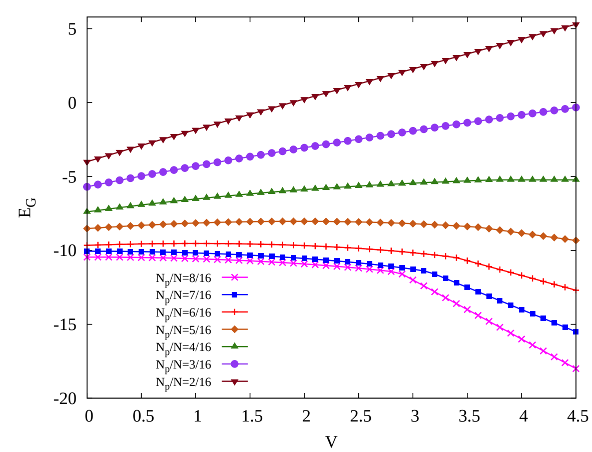

FIG. 3. (Color online) Plots of energy E_G (obtained using modified Lanczos in a system with $N = 16$ sites) for the extremely anisotropic NNN Heisenberg model at various magnetizations $(N - 2N_p)/N$ corresponding to fillings $\mathrm{f} = N_p/N$ for the $t_2 - V$ model.

III. ANALYSIS OF THE HALF-FILLED $t_2 - V$ MODEL

We study the following $t_2 - V$ Hamiltonian in rings with even number of sites by considering two sublattices C and D and using periodic boundary conditions:

$$\begin{aligned} H \equiv & -t_2 \sum_{i=1}^{N/2} (c_i^\dagger c_{i+1} + \text{H.c.}) \\ & -t_2 \sum_{i=1}^{N/2} (d_i^\dagger d_{i+1} + \text{H.c.}) \\ & +V \sum_{i=1}^{N/2} d_i^\dagger d_i (c_i^\dagger c_i + c_{i-1}^\dagger c_{i-1}), \end{aligned} \tag{13}$$

where c and d denote destruction operators of HCBs in sublattices C and D, respectively. To understand the striking discontinuous phase transition at half-filling, (i.e., the transition from equal occupation of both sublattices to occupation of only one sublattice at a critical V_c) we begin by recognizing that when the system is on the verge of completing the phase transition, the system will pass through the state where there is one particle in one sublattice and one hole in the other sublattice. Hence, we now consider instability for the case of one particle in sublattice C and one hole [with destruction operator denoted by h ($\equiv d^\dagger$)] in sublattice D; we then rearrange the above equation as

$$\begin{aligned} H \equiv & -t_2 \sum_{i=1}^{N/2} (c_i^\dagger c_{i+1} + \text{H.c.}) \\ & +t_2 \sum_{i=1}^{N/2} (h_i^\dagger h_{i+1} + \text{H.c.}) \\ & -V \sum_{i=1}^{N/2} (h_i^\dagger h_i - 1)(c_i^\dagger c_i + c_{i-1}^\dagger c_{i-1}). \end{aligned} \tag{14}$$

We define the particle-hole Green's function as follows[25]:

$$g_n^h \equiv {}_h\langle k, 0|G(\omega)|k, n\rangle_h, \tag{15}$$

where

$$G(\omega) \equiv \frac{1}{(\omega + i\eta - H)}, \tag{16}$$

and the particle-hole state $|k, n\rangle_h$

$$|k, n\rangle_h = \frac{1}{\sqrt{N}} \sum_{i=1}^{N/2} e^{ik\left(R_i + \frac{na}{2}\right)} c_i^\dagger h_{i+n}^\dagger |0\rangle, \tag{17}$$

with k being the total momentum of the particle-hole system, na the separation between the particle and hole, and a the lattice constant of a sublattice. Using the condition

$$\delta_{0,n} \equiv {}_h\langle k, 0|G(\omega)(\omega + i\eta - H)|k, n\rangle_h, \tag{18}$$

for $n = 0$, we obtain

$$\begin{aligned} (\omega + i\eta) g_0^h &= 1 + {}_h\langle k, 0|G(\omega)(H)|k, 0\rangle_h \\ &= 1 + V g_0^h - i2t_2 \sin(ka/2) g_1^h \\ &\quad + i2t_2 \sin(ka/2) g_{-1}^h. \end{aligned} \tag{19}$$

From Eq. (18), for $n = 1$, we get

$$\begin{aligned} (\omega + i\eta) g_1^h &= {}_h\langle k, 0|G(\omega)(H)|k, 1\rangle_h \\ &= V g_1^h - i2t_2 \sin(ka/2) g_2^h \\ &\quad + i2t_2 \sin(ka/2) g_0^h. \end{aligned} \tag{20}$$

Similarly, for $n \neq 0, 1$, we derive

$$\begin{aligned} (\omega + i\eta) g_n^h &= {}_h\langle k, 0|G(\omega)(H)|k, n\rangle_h \\ &= 2V g_n^h - i2t_2 \sin(ka/2) g_{n+1}^h \\ &\quad + i2t_2 \sin(ka/2) g_{n-1}^h. \end{aligned} \tag{21}$$

As V increases to the critical interaction V_c, the energy given by Eq. (13) becomes 0 (i.e., energy of all HCBs filling up one sublattice). This would correspond to the level-crossing instability [in the system represented by Eq. (14)] where the particle HCB quits its sublattice and goes into the sublattice of the hole.

Now, let

$$\frac{\omega + i\eta - 2V}{F_k} \equiv \frac{1}{z} - z, \tag{22}$$

where $F_k \equiv i2t_2 \sin(ka/2)$. Then, Eq. (21) takes the simple form

$$\left(\frac{1}{z} - z\right) g_n^h = g_{n-1}^h - g_{n+1}^h, \tag{23}$$

whose solution is of the form

$$g_n^h = \alpha_1^\pm z^n + \frac{\beta_1^\pm}{(-z)^n}, \tag{24}$$

where α_1^+ (α_1^-) and β_1^+ (β_1^-) correspond to $n > 1$ ($n < 0$). The transition occurs at the critical value of V that makes the overall energy 0. Let $V = 2t_2\gamma \sin(ka/2)$. The overall energy is less than $-4t_2+2V$ (for $V > 0$). It is important to note that, for the groundstate, $k = \pi/a$ for any V. This can be seen by first noting that when $V = 0$, total momentum in the minimum energy state is π/a; next, turning on V does not change the total momentum. Then for $k = \pi/a$, to get overall energy to be 0, we need the inequality $\gamma > 1$. To get the instability condition, we consider the case $\omega = 0$ so that the Green's function g_0^h diverges at the transition point. It then follows from Eq. (22) that

$$i2\gamma = \frac{1}{z} - z, \tag{25}$$

which implies that

$$z = i(-\gamma + \sqrt{\gamma^2 - 1}), \tag{26}$$

and hence $|z| < 1$ for $\gamma > 1$. Let us first consider the case $n > 1$. From the above Eq. (24), it is clear that, for $n \to \infty$, g_n^h is finite only for $\beta_1^+ = 0$. Thus for $n > 1$,

$$g_{n+1}^h = z g_n^h, \tag{27}$$

which implies that $g_3^h = z g_2^h$; then, from Eq. (23) it follows that

$$g_2^h = z g_1^h. \tag{28}$$

Next, for the case $n < 0$, we see that g_n^h is finite, for $n \to -\infty$, only when $\alpha_1^- = 0$. Thus for $n < 0$,

$$g_{n-1}^h = -z g_n^h, \tag{29}$$

which implies that $g_{-2}^h = -z g_{-1}^h$; then from Eq. (23) we obtain

$$g_{-1}^h = -z g_0^h. \tag{30}$$

From Eqs. (19), (20), (28), and (30), we obtain

$$g_0^h = \frac{1}{(\omega + i\eta - V + zF_k) + \frac{F_k^2}{(\omega + i\eta - V + zF_k)}}, \tag{31}$$

and

$$g_1^h = \frac{g_0^h F_k}{(\omega + i\eta - V + zF_k)}, \tag{32}$$

where $\omega = 0$, $V = 2t_2\gamma$, $z = i(-\gamma + \sqrt{\gamma^2 - 1})$, and $F_k = i2t_2$. It then follows that g_0^h diverges when $(V - zF_k)^2 + F_k^2 = 0$, i.e., when $\gamma = \sqrt{2}$. Thus the instability condition is $V_c = 2\sqrt{2}t_2$. (We now see that the total energy at transition is indeed less than $-4t_2 + 2V$). It is important to note [as can be seen from Eq. (32)] that, when g_0^h diverges, g_1^h also diverges; consequently, from Eqs. (27), (29), and (30) we see that all g_n^h diverge (i.e., even when $n > 1$ and $n < 0$).

IV. TWO HCBS IN $t_2 - V$ MODEL

We study the $t_2 - V$ Hamiltonian [described by Eq. (13)] in rings with even number of sites and for periodic boundary conditions. We consider one HCB in sublattice C and one HCB in sublattice D; the corresponding two-particle Green's function is defined by

$$g_n \equiv \langle k, 0|G(\omega)|k, n\rangle, \tag{33}$$

where $G(\omega)$ is given by Eq. (16) and the two-particle state $|k, n\rangle$ is defined as

$$|k, n\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^{N/2} e^{ik\left(R_i + \frac{na}{2}\right)} c_i^\dagger d_{i+n}^\dagger |0\rangle, \tag{34}$$

with k representing the total momentum of the two-particle system. Then, the following equations hold for the Green's functions g_n:

$$\begin{aligned}(\omega + i\eta - V)g_0 = 1 &- 2t_2 \cos(ka/2) g_1 \\ &-2t_2 \cos(ka/2) g_{-1},\end{aligned} \tag{35}$$

$$\begin{aligned}(\omega + i\eta - V)g_1 = &-2t_2 \cos(ka/2) g_2 \\ &-2t_2 \cos(ka/2) g_0,\end{aligned} \tag{36}$$

and for $n \neq 0, 1$

$$\begin{aligned}(\omega + i\eta)g_n = &-2t_2 \cos(ka/2) g_{n+1} \\ &-2t_2 \cos(ka/2) g_{n-1}.\end{aligned} \tag{37}$$

As V increases to the critical V_c, the energy given by Eq. (13) becomes $-4t_2 \cos(2\pi/N)$ (i.e., the minimum energy of 2 HCBs in the same sublattice); this would correspond to the instability for Eq. (13) where one HCB quits its sublattice and goes into the sublattice of the other particle. Here, we make the key observation that $k = 0$ for the groundstate at any V; to understand this, we first note for $V = 0$, the total momentum is zero in the minimum energy state; next, we recognize that turning on V does not change the total momentum.

Now, to obtain the instability , we take

$$\begin{aligned}\frac{\omega}{(-2t_2)} &= \frac{4t_2 \cos(2\pi/N)}{2t_2} = 2\cos(2\pi/N) \\ &= e^{i2\pi/N} + e^{-i2\pi/N} \\ &= z + \frac{1}{z}.\end{aligned} \tag{38}$$

We set $z = e^{i2\pi/N}$ and assume $\eta \to 0$ faster than $\sin(2\pi/N)$ as $N \to \infty$ in the thermodynamic limit. We also take $V/(2t_2) = 2\gamma$. Then Eqs. (35), (36), and (37) become

$$[(z + 1/z) + 2\gamma]g_0 = -1/(2t_2) + g_1 + g_{-1}, \tag{39}$$

$$[(z + 1/z) + 2\gamma]g_1 = g_2 + g_0, \tag{40}$$

and for $n \neq 0, 1$

$$[(z + 1/z)]g_n = g_{n+1} + g_{n-1}. \tag{41}$$

Without loss of generality, we assume

$$g_1 = \alpha_2 z + \beta_2/z, \tag{42}$$

and

$$g_2 = \alpha_2 z^2 + \beta_2/z^2. \tag{43}$$

Then using Eqs. (41), (42), and (43), we obtain for $n = 3, 4, ..., N/2$ the expression

$$g_n = \alpha_2 z^n + \beta_2/z^n. \tag{44}$$

It is important to note that $|z| = 1$ and hence the Green's functions do not decay with n! From the fact that at two-particle momentum $k = 0$, $|k, n\rangle = |k, n - N/2\rangle$, we see that $g_{\frac{N}{2}} = g_0$ and $g_{\frac{N}{2}-1} = g_{-1}$. Then, using Eq. (44) and the relation $z = e^{i2\pi/N}$, we get

$$\begin{aligned}g_{-1} = g_{\frac{N}{2}-1} &= \alpha_2 z^{\frac{N}{2}-1} + \beta_2/z^{\frac{N}{2}-1} \\ &= -(\alpha_2/z + \beta_2 z),\end{aligned} \tag{45}$$

and

$$g_0 = g_{\frac{N}{2}} = \alpha_2 z^{\frac{N}{2}} + \beta_2/z^{\frac{N}{2}} \\ = -(\alpha_2+\beta_2). \quad (46)$$

We are now ready to solve for the Green's functions g_n using Eqs. (39), (40), (42), (43), (45), and (46). We get the following equations:

$$\alpha_2[z+\gamma] + \beta_2[1/z+\gamma] = 1/(4t_2), \quad (47)$$

and

$$\alpha_2[1+\gamma z] + \beta_2[1+\gamma/z] = 0. \quad (48)$$

It then follows from the above two equations that

$$\alpha_2 = \frac{z+\gamma}{4t_2(z^2+\gamma^2-1-\gamma^2 z^2)}, \quad (49)$$

which diverges when $\gamma = \pm 1$. We choose $\gamma = 1$ for repulsive V. Furthermore,

$$\beta_2 = -\alpha_2 \frac{1+\gamma z}{1+\gamma/z}, \quad (50)$$

which for $\gamma = 1$ yields $\beta_2 = -\alpha_2 z$. Thus we see that $g_0 = -(\alpha_2+\beta_2) = -\alpha_2(1-z)$ diverges for $\gamma = 1$ or $V_c = 4t_2$. We also find that for $0 \neq n \leq \frac{N}{2}$

$$g_n = \alpha_2 z^n + \beta_2/z^n = \alpha_2\left(e^{i2\pi n/N} - e^{-i2\pi(n-1)/N}\right), \quad (51)$$

also diverges since $2n-1 \neq N$. *The instability/divergence condition $V_c = 4t_2$ is independent of N and hence is valid in the thermodynamic limit as well!* Another interesting observation based on $\beta_2 = -\alpha_2 z$ is that

$$g_{-k} = g_{\frac{N}{2}-k} = -\alpha_2/z^k - \beta_2 z^k \\ = \beta_2/z^{k+1} + \alpha_2 z^{k+1} \\ = g_{k+1}. \quad (52)$$

V. CONCLUSIONS

In the $t_2 - V$ model, for $V >> t_2$, energy considerations show that the system always has only one sublattice populated for less than half-filling[1]. Additionally, we demonstrate that our $t_2 - V$ model undergoes a dramatic first-order QPT at non-half-fillings from a superfluid to a supersolid state with homogeneously coexisting $U(1)$ symmetry broken superfluid and a period-doubling CDW. Using two-particle Green's functions we derive the QPT condition exactly for the half-filled case and the instability condition for the 2 HCB case for all system sizes. The model studied is a limiting case of the strong electron-phonon coupling in one-dimensional systems with cooperative breathing mode. A similar analysis in two-dimensions is left for future studies.

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Appendix A: Finite size scaling analysis for HCBs in $t_2 - V$ model

In this appendix, we will outline our approach to carrying out finite size scaling analysis. Let us first consider a non-interacting system (with N sites and N_p particles) described by a tight-binding Hamiltonian. For even number of particles, the ground state has particles occupying momenta $\frac{(2m+1)\pi}{Na}$ with $-N_p/2 \leq m \leq N_p/2-1$; whereas for odd number of particles the ground state is represented by particle momenta $\frac{(2m)\pi}{Na}$ with $-(N_p-1)/2 \leq m \leq (N_p-1)/2$. Thus the ground state wavefunction (due to the occupied momenta) is an even function of $1/N$. Hence, for the case corresponding to after the phase transition where all the particles are in the same sublattice C, the energy of the ground state $|\phi_0\rangle$ is given by

$$E_I = \sum_{i=1}^{N/2} \langle\phi_0| - t_2(c_i^\dagger c_{i+1} + \text{H.c.})|\phi_0\rangle, \quad (A1)$$

where c is the destruction operator for a HCB in sublattice C. Upon taking into account discrete translational symmetry, we get

$$\frac{2E_I}{N} = \langle\phi_0| - t_2(c_i^\dagger c_{i+1} + \text{H.c.})|\phi_0\rangle. \quad (A2)$$

Since $|\phi_0\rangle$ is even in $1/N$, we note that $\frac{E_I}{N}$ is also even in $1/N$.

Next, consider the interacting system characterized by the following $t_2 - V$ Hamiltonian in rings with even number of sites (N) and with periodic boundary conditions:

$$H \equiv -t_2 \sum_{i=1}^{N/2}(c_i^\dagger c_{i+1} + \text{H.c.}) \\ -t_2 \sum_{i=1}^{N/2}(d_i^\dagger d_{i+1} + \text{H.c.}) \\ +V \sum_{i=1}^{N/2} d_i^\dagger d_i (c_i^\dagger c_i + c_{i-1}^\dagger c_{i-1}), \quad (A3)$$

where c (d) is the destruction operator for HCB in sublattice C (D)and $V \geq 0$. Upon invoking reflection symmetry, we note that the ground state will be invariant when the sign of momenta is reversed; equivalently the ground state $|\psi_0\rangle$ is an even function of $1/N$. The ground

state energy, before the phase transition, is given by

$$E_{II} = \sum_{i=1}^{N/2} \langle\psi_0| - t_2[(c_i^\dagger c_{i+1} + \text{H.c.}) + (d_i^\dagger d_{i+1} + \text{H.c.})]|\psi_0\rangle + \sum_{i=1}^{N/2} \langle\psi_0|V d_i^\dagger d_i (c_i^\dagger c_i + c_{i-1}^\dagger c_{i-1})|\psi_0\rangle. \tag{A4}$$

Upon recognizing discrete translational invariance, we see that

$$\frac{2E_{II}}{N} = \langle\psi_0| - t_2[(c_i^\dagger c_{i+1} + \text{H.c.}) + (d_i^\dagger d_{i+1} + \text{H.c.})]|\psi_0\rangle + \langle\psi_0|V d_i^\dagger d_i (c_i^\dagger c_i + c_{i-1}^\dagger c_{i-1})|\psi_0\rangle. \tag{A5}$$

Since, $|\psi_0\rangle$ is even in $1/N$, it follows that $\frac{E_{II}}{N}$ is also even in $1/N$.

Now, at the transition point (corresponding to a critical interaction V_c), $\frac{E_{II}}{N} - \frac{E_I}{N} = 0$; this implies that

$$V_c = \frac{\langle\psi_0|t_2[(c_i^\dagger c_{i+1} + \text{H.c.}) + (d_i^\dagger d_{i+1} + \text{H.c.})]|\psi_0\rangle}{\langle\psi_0|d_i^\dagger d_i (c_i^\dagger c_i + c_{i-1}^\dagger c_{i-1})|\psi_0\rangle} - \frac{\langle\phi_0|t_2(c_i^\dagger c_{i+1} + \text{H.c.})|\phi_0\rangle}{\langle\psi_0|d_i^\dagger d_i (c_i^\dagger c_i + c_{i-1}^\dagger c_{i-1})|\psi_0\rangle}. \tag{A6}$$

In the above equation, because both numerator and denominator of all the terms on the right-hand side are even in $1/N$, it follows that V_c is also even in $1/N$.

It is also important to note that we used general arguments to show that the ground state energy $\frac{E_{II}}{N}$ is even in $1/N$; these arguments can be extended to show that the ground state energies of other interacting systems such as the $t - V$ model are also even functions of $1/N$.

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